C
Chem 4100
Questions from Exam II Fall 2015
Instrumental Analysis: IR, Raman, and NMR

Dr. Stone
Name_________________________

Some useful information:

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Magnetogyric ratio (radian/T*sec), T=Tesla</th>
<th>Isotope abundance</th>
<th>Relative sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>¹H</td>
<td>2.88 x 10⁸</td>
<td>99.98</td>
<td>1.00</td>
</tr>
<tr>
<td>¹³C</td>
<td>6.73 x 10⁷</td>
<td>1.11</td>
<td>0.016</td>
</tr>
</tbody>
</table>

Equations and Constants

\[ c = 2.99792 \times 10^8 \text{ m/sec} \]
\[ k = 1.38065 \times 10^{-23} \text{ J/K} \]
\[ eV=1.692 \times 10^{-19} \text{ J} \]
\[ h=6.626 \times 10^{-34} \text{ J*sec} \]

- \( v = c/\lambda \)
- \( v = v/\lambda \)
- \( v = c/n \)
- \( \sin \theta_1 = n_2 \)
- \( \sin \theta_2 = n_1 \)
- \( n\lambda = d (\sin i + \sin r) \)

\[ \Delta \nu = \frac{1}{\delta} P(\delta) = \frac{1}{2} P(\nu) \cos 2\pi ft \]
\[ f = \frac{2\nu_M}{c} \]

1. (10 points) The following molecular stretches may or may not be IR active. Number the IR active stretches in order of increasing wavenumber. The stretch with the lowest wavenumber will be number one. For the stretches that are not IR active, briefly state why.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Stretch</th>
</tr>
</thead>
<tbody>
<tr>
<td>Propane</td>
<td>asymmetric C-H stretch (methyl)</td>
</tr>
<tr>
<td>Ethylene</td>
<td>symmetric C=C stretch</td>
</tr>
<tr>
<td>Formaldehyde (CH₂O)</td>
<td>symmetric C=O stretch</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>symmetric C=O stretch</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>bend</td>
</tr>
<tr>
<td>Ozone, (O₃)</td>
<td>symmetric O-O stretch</td>
</tr>
<tr>
<td>Nitric oxide (NO)</td>
<td>N=O stretch</td>
</tr>
<tr>
<td>Nitrogen gas</td>
<td>N≡N stretch</td>
</tr>
</tbody>
</table>
2. (20 points) Fully describe how a Michelson interferometer is used in an FTIR instrument. Express your answer in complete sentences organized into paragraph form. Use drawings when appropriate, and be sure to label everything clearly.
3. (10 points) For the following spectrum of methyl benzoate, draw the structure and assign the major peaks in the IR spectrum:

![IR Spectrum of Methyl Benzoate](image)

4. (5 points) Briefly describe Raman spectroscopy. How is it similar to IR spectroscopy? How is it different?

5. (25 points) NMR instruments are named by the frequency of a proton’s resonance in the magnetic field. The chemistry department has a 500 MHz instrument. Some chemistry departments have 600 MHz instruments.
   a. What is the magnetic field strength (in Tesla) of a magnet, if protons with no shielding resonate at 500MHz?
   b. The cost of a 500 MHz instrument is about 30% less than the cost of a 600 MHz instrument. Also, the 600MHz magnet requires more expensive liquid helium and liquid nitrogen to cool the superconducting magnet. Describe the advantages of having a 600 MHz instrument.
   c. The methylene protons in 3-methyl-1-butanol resonate at 4.99999250 x 10^8 Hz in a 500 MHz instrument, their chemical shift is 1.5ppm in the 500MHz instrument. What is the chemical shift for these same protons in a 300 MHz instrument?
   d. In general why do more electron withdrawing groups cause a signal to appear at a higher frequency, (more down field).
   e. Why is $^{13}$C much less sensitive?
   f. What two things can be done to increase the signal to noise for $^{13}$C? How does each of these increase the signal?
6. (20 points) Given the following $^1$H and $^{13}$C spectra (in CDCl$_3$), determine the structure for a compound with the formula C$_5$H$_{12}$O. Give the IUPAC name for this compound and draw the structure. Also, assign the peaks on both spectra. The peak at 2.8 ppm is a proton bonded to an oxygen.

7. Draw the expected COSY spectrum for your structure of C$_5$H$_{12}$O that you determined in the previous experiment.